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Models of the Pseudogap State in Cuprates

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We review a certain class of ("nearly") exactly solvable models of electronic spectrum of two-dimensional systems with fluctuations of short range order of "dielectric" (e.g. antiferromagnetic) or "superconducting" type, leading to the formation of anisotropic pseudogap state on certain parts of the Fermi surface. The models are based on recurrence procedure for one- and two-electron Green's functions which takes into account of all Feynman diagrams in perturbation series with the use of the approximate Ansatz for higher-order terms in this series. These models can be applied to calculation of spectral density, density of states and conductivity in the normal state, as well as to calculation of some properties of superconducting state.

The model of "nearly – antiferromagnetic" Fermi-liquid is based upon the picture of well developed fluctuations of AFM short range order in a wide region of the phase diagram. In this model the effective interaction of electrons with spin fluctuations is described via dynamic spin susceptibility $\chi_{\mathbf{q}}(\omega)$, which is determined mainly from the fit to NMR experiments [1]:

$$V_{eff}(\mathbf{q},\omega) = g^2\chi_{\mathbf{q}}(\omega) \approx \frac{g^2\xi^2}{1+\xi^2(\mathbf{q}-\mathbf{Q})^2 - i\frac{\omega}{\omega_{sf}}} \quad (1)$$

where g is coupling constant, ξ–correlation length of spin fluctuations, $\mathbf{Q} = (\pi/a, \pi/a)$–vector of antiferromagnetic ordering in insulating phase, ω_{sf}–characteristic frequency of spin fluctuations, a–lattice spacing. As dynamic spin susceptibility $\chi_{\mathbf{q}}(\omega)$ has peaks at the wave vectors around $(\pi/a, \pi/a)$ there appear "two types" of quasiparticles — "hot quasiparticles" with momenta in the vicinity of "hot spots" on the Fermi surface and "cold" quasiparticles with momenta on the other parts of the Fermi surface, e.g. around diagonals of the Brillouin zone $|p_x| = |p_y|$ [1].

In the following we shall consider the case of high enough temperatures when $\pi T \gg \omega_{sf}$ which corresponds to the region of "weak pseudogap" [1]. In this case spin dynamics is irrelevant and we can limit ourselves to static approximation.

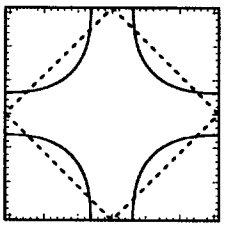

Figure 1. "Hot spots" model. Electronic states around the intersection points of the Fermi surface with magnetic Brillouin zone (shown by dashed lines) are strongly interacting with fluctuations of AFM short range order.

We can greatly simplify all calculations if instead of (1) we use another form of model interaction:

$$V_{eff}(\mathbf{q}) = \Delta^2 \frac{2\xi^{-1}}{\xi^{-2}+(q_x-Q_x)^2} \frac{2\xi^{-1}}{\xi^{-2}+(q_y-Q_y)^2} \quad (2)$$

where Δ is some phenomenological parameter, determining the effective width of the pseudogap. In fact (2) is qualitatively similar to the static limit of (1) and differs from it very slightly in most important region of $|\mathbf{q}-\mathbf{Q}| < \xi^{-1}$.

The spectrum of "bare" (free) quasiparticles

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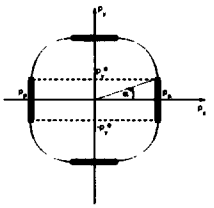

Figure 2. Model of the Fermi surface for HTSC-cuprates. "Hot patches" are shown by thick lines of the width of ξ^{-1}).

can be taken in the form [1]:

$$\xi_{\mathbf{p}} = -2t(\cos p_x a + \cos p_y a) - 4t' \cos p_x a \cos p_y a \quad (3)$$

where t–nearest neighbor transfer integral, a t'–second nearest neighbor transfer integral on the square lattice, μ is chemical potential.

Much simpler model of electronic spectrum assumes that the Fermi surface of two – dimensional system to have nesting ("hot") patches of finite angular size α in $(0,\pi)$ and symmetric directions in the Brillouin zone, as shown in Fig.2 [6]. Similar Fermi surface was observed in a number of ARPES experiments on cuprate superconductors. Here we assume that fluctuations interact only with electrons from the "hot" (nesting) patches of the Fermi surface, and scattering vector is either $Q_x = \pm 2p_F$, $Q_y = 0$ or $Q_y = \pm 2p_F$, $Q_x = 0$ for incommensurate fluctuations, while $\mathbf{Q} = (\pi/a, \pi/a)$ for commensurate case. It is easily seen that this scattering is in fact of one – dimensional nature. In this case non-trivial contributions of interaction with fluctuations appear only for electrons from "hot" patches, while electrons on "cold" parts of the Fermi surface remain free.

These models can be solved exactly in the limit of infinite correlation length $\xi \to \infty$, using methods developed in Refs. [2,3]. For the case of finite ξ we can use an approximate Ansatz, proposed for one – dimensional case in Ref. [4] and further developed for two – dimensional system in Refs. [1,7]. According to this Ansatz the contribution of an arbitrary diagram for electron self-energy of N-th order in interaction (2) has the form:

$$\Sigma^{(N)}(\varepsilon_n \mathbf{p}) = \Delta^{2N} \prod_{j=1}^{2N-1} \frac{1}{i\varepsilon_n - \xi_j + i n_j v_j \kappa} \quad (4)$$

where for the "hot spots" model $\xi_j = \xi_{\mathbf{p}+\mathbf{Q}}$ and $v_j = |v^x_{\mathbf{p}+\mathbf{Q}}| + |v^y_{\mathbf{p}+\mathbf{Q}}|$ for odd j and $\xi_j = \xi_{\mathbf{p}}$ and $v_j = |v^x_{\mathbf{p}}| + |v^y_{\mathbf{p}}|$ for even j – appropiate combinations of velocity projections, determined by the "bare" spectrum (3). For the "hot patches" model $\xi_j = (-1)^j \xi_{\mathbf{p}}$, $v_j = v_F$. Here n_j is the number of interaction lines, enveloping j-th Green's function in a given diagram. In this case any diagram with intersecting interaction lines is actually equal to some diagram of the same order with noncrossing interaction lines. Thus in fact we can consider only diagrams with nonintersecting interaction lines, taking into account diagrams with intersecting lines introducing additional combinatorial factors into interaction vertices. This method was used for one-dimensional model of the pseudogap state in Refs. [4,5].

As a result we obtain the following recursion relation for one-electron Green's function (continuous fraction representation) [4,5,7]:

$$G^{-1}(\varepsilon_n \xi_{\mathbf{p}}) = G_0^{-1}(\varepsilon_n \xi_{\mathbf{p}}) - \Sigma_1(\varepsilon_n \xi_{\mathbf{p}}) \quad (5)$$

$$\Sigma_k(\varepsilon_n \xi_{\mathbf{p}}) = \Delta^2 \frac{v(k)}{i\varepsilon_n - \xi_k + ikv_k\kappa - \Sigma_{k+1}(\varepsilon_n \xi_{\mathbf{p}})} \quad (6)$$

Combinatorial factor:

$$v(k) = k \quad (7)$$

corresponds to the case of commensurate fluctuations with $\mathbf{Q} = (\pi/a, \pi/a)$ [4]. For incommensurate case [4]:

$$v(k) = \begin{cases} \frac{k+1}{2} & \text{for odd } k \\ \frac{k}{2} & \text{for even } k \end{cases} \quad (8)$$

In Ref. [1] a spin-structure of effective interaction within the model of "nearly antiferromagnetic" Fermi-liquid was taken into account (spin-fermion model). This leads to more complicated combinatorics of diagrams. Spin-conserving part of the

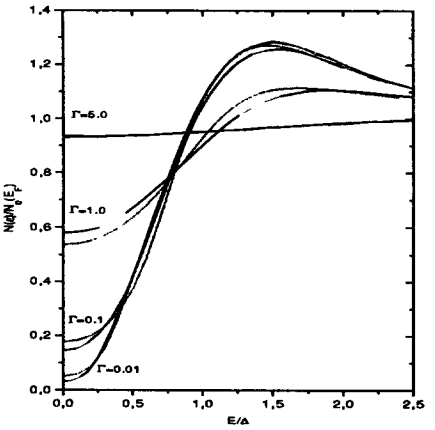

Figure 3. Density of states in one – dimensional version of the model for incommensurate case and different values of $\Gamma = v_F\kappa/\Delta$. Full lines – exact numerical diagonalization (data of Ref.[9]), dotted lines – our Ansatz.

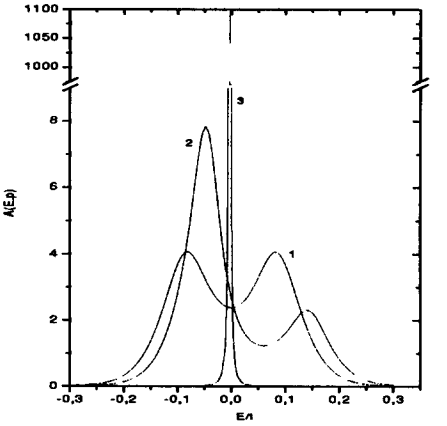

Figure 4. Energy dependencies of spectral density for $\kappa a = 0.01$, $t'/t = -0.4$, $\mu/t = -1.3$. Incommensurate case. (1)—at the "hot spot" $p_x a/\pi = 0.142$, $p_y a/\pi = 0.857$. (2)—close to the "hot spot" $p_x a/\pi = 0.145$, $p_y a/\pi = 0.843$. (3)—far from the "hot spot" $p_x a/\pi = p_y a/\pi = 0.375$.

interaction gives formally commensurate combinatorics, while spin-flip scattering is described by diagrams with combinatorics of incommensurate type. In this case [1]:

$$v(k) = \begin{cases} \frac{k+2}{3} & \text{for odd } k \\ \frac{k}{3} & \text{for even } k \end{cases} \qquad (9)$$

This approach was generalized for calculation of two – electron Green's function in Ref. [5], where we formulated some recursion relations for the vertex part, describing electronic response to an external electromagnetic field, allowing calculations of conductivity.

The Ansatz of (4) is in fact not precisely exact [8], however the analysis of Ref. [7], shows that it is quantitatively good for most interesting cases. These conclusions were confirmed in recent papers [9,10], where the one – dimensional version of our model was solved by exact numerical diagonalization. In Fig.3 we show the comparison of results obtained for the density of states in case of incommensurate fluctuations by exact numerics [9] and via our recursion relations. We can see an extremely good correspondence, sufficient for any practical purposes. In case of commensurate fluctuations in one – dimension the Ansatz of (4) misses certain Dyson type singularity of the density of states, appearing at the center of the pseudogap [9,10], but this is apparently absent in two – dimensional case.

Consider one-electron spectral density:

$$A(E\mathbf{p}) = -\frac{1}{\pi} Im G^R(E\mathbf{p}) \qquad (10)$$

where $G^R(E\mathbf{p})$ is retarded Green's function, obtained by the usual analytic continuation of (5) to the real axis of energy E. In Fig.4 we show typical energy dependencies of $A(E\mathbf{p})$ obtained for the "hot spots" model. More detailed results can be found in Refs. [1,7]. Similar non Fermi – liquid like behavior of the spectral density is easily obtained on "hot patches" of the Fermi surface shown in Fig.2 (Cf. Ref. [5]).

Let us stress that our solution (6) is exact both for $\xi \to \infty$ and $\xi \to 0$, while in the region of finite ξ it provides apparently very good interpolation.

The one-electron density of states:

$$N(E) = \sum_{\mathbf{p}} A(E,\mathbf{p}) = -\frac{1}{\pi}\sum_{\mathbf{p}} ImG^R(E\mathbf{p}) \quad (11)$$

is determined by the integral of spectral density $A(E\mathbf{p})$ over the Brillouin zone. Detailed results for the "hot spots" model were obtained in Ref. [7], demonstrating smeared pseudogap with weak dependence on the correlation length ξ. For "hot patches" model this pseudogap is more pronounced, depending on the size of these patches.

"Hot patches" model was applied by us to calculations of optical conductivity [11] and also (for the simplest case of $\xi \to \infty$) to the study of the main superconducting properties [6,12].

Pseudogap phenomena can also be explained using the idea of fluctuation Cooper pairing at temperatures higher than superconducting transition temperature T_c. Anticipating the possibility of both s-wave and d-wave pairing, we introduce the pairing interaction of the simplest (separable) form:

$$V(\mathbf{p},\mathbf{p}') = -Ve(\phi)e(\phi') \quad (12)$$

where ϕ is polar angle determining the direction of electronic momentum $\mathbf{p}$ in the plane, while for $e(\phi)$ we assume model dependence:

$$e(\phi) = \begin{cases} 1 & s\text{-wave pairing} \\ \sqrt{2}\cos(2\phi) & d\text{-wave pairing} \end{cases} \quad (13)$$

Analogously to transition from (1) to (2) we introduce the model interaction (static fluctuation propagator of Cooper pairs):

$$V_{eff}(\mathbf{q}) = -\Delta^2 e^2(\phi)\frac{2\xi^{-1}}{\xi^{-2}+q_x^2}\frac{2\xi^{-1}}{\xi^{-2}+q_y^2} \quad (14)$$

where Δ determines the width of superconducting pseudogap. We can see that mathematically this problem is practically the same as the "hot spot" model, but always with combinatorics of incommensurate case [7]. Then we again obtain the recurrence relation for the Green's function of the type of (6):

$$\Sigma_k(\varepsilon_n\xi\mathbf{p}) = \frac{\Delta^2 e^2(\phi)v(k)}{i\varepsilon_n - (-1)^k\xi\mathbf{p} + ik(|v_x|+|v_y|)\kappa - \Sigma_{k+1}(\varepsilon_n\xi\mathbf{p})} \quad (15)$$

where $v_x = v_F\cos\phi$, $v_y = v_F\sin\phi$, $\kappa = \xi^{-1}$, $\varepsilon_n > 0$ and $v(k)$ was defined in (8).

Energy dependencies of the spectral density $A(E\mathbf{p})$ for one-particle Green's function (10), can be calculated from (15) for different values of polar angle ϕ, determining the direction of electronic momentum in the plane, for the case of fluctuations of d-wave pairing. Calculations show [7] that in the vicinity of the point $(\pi/a, 0)$ in Brillouin zone this spectral density is non Fermi-liquid like (pseudogap behavior). As vector $\mathbf{p}$ rotates in the direction of the zone diagonal the two peak structure gradually disappears and spectral density transforms to the typical Fermi-liquid like with a single peak, which narrows as ϕ approaches $\pi/4$. Analogous transformation of the spectral density takes place as correlation length ξ becomes smaller. In case of fluctuation pairing of s-wave type the pseudogap appears isotropically on the whole Fermi-surface.

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